Inertance Tube and Reservoir Modeling: Meshing, Convergence and Friction Factors for Oscillating Flow

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ABSTRACT

Pulse tube refrigerators (PTRs) have made dramatic improvements in reliability, efficiency and usage, with the addition of the inertance tube helping to create the improvements. The combination of the inertance tube and reservoir help to create a phase shift between mass flow rate and pressure that affects the fluid dynamics in the PTR. Current models inadequately predict (in accuracy) the phase shifts in these oscillating refrigerators. Various modeling techniques have yet to address the issue of numerical solution convergence, especially with respect to the mesh size and time step size when using Computational Fluid Dynamics (CFD) models. This study aims to address the issue based on comparisons to a set of experimental results. Along with the CFD correlation, a comparison with a distributed inertance tube model based on new friction factors for oscillating flow will be reported. A comparison of isothermal to mixed surface wall boundary condition is performed.

INTRODUCTION

Pulse Tube Refrigerators (PTRs) play an important role in satisfying the need for cryogenic cooling of many applications where high reliability, low vibration, and high efficiency are requirements. The most promising technology to create more efficient PTRs is the phase shifter,[1-4] which controls the phase shift between the mass flow rate and the pressure. One phase shifter with a very promising ability to effect efficiency is the inertance tube.[1,5,6] Figure 1 shows the main components of an Inertance Tube PTR (ITPTR).

Various models for designing cryocoolers exist, from first order models to higher order models such as CFD calculations for predictions of flows in the cryocooler's components. In first-order models, usually used in design analysis and parametric studies of ITPTRs, a lumped parameter approximation is used to take into account the inertance, compliance, and the fluid flow resistance associated with the oscillating flow in the inertance tube. In the previous studies,[7,8] a convenient correlation for the entire range of laminar and turbulent flow is used with a modified distributed component model[5,6] and was integrated with REGEN3.2 and a parametric model for pulse tube inefficiencies. As was shown in the last study, the acoustic power and phase shift as calculated from the CFD results only nominally compared to the experimental data. Since no error bars were calculated for the CFD calculations it was hard to determine if the lack of correlation was due to the simulation set up, the experimental set up, or the input uncertainty. The distributed model is used to

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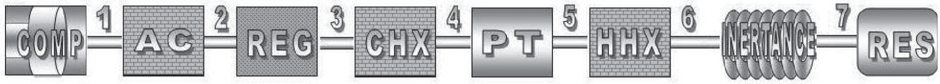

Figure 1. Inertance Tube Pulse Tube Refrigerator (ITPTR)

model the inertance tube, and to compare to the CFD simulations[7] and to previously published experimental data.[9] The distributed component method divides the inertance tube into several sections and applies the lumped parameter model to each section.[1,7]

This study expands on previous studies, by comparing the previous studies' model where (1) the reservoir is not meshed and is simulated with equations[8] and (2) implement a user defined function in the CFD software Fluent™. In this study the reservoir is fully meshed and comparisons are made to the user defined function. Grid convergence studies were performed on both inertance tubes with meshed reservoirs and with inertance tubes with the user defined reservoir function to quantify errors associated with using the CFD software. All of the previously mentioned simulations assumed isothermal boundary conditions for both the inertance tube and reservoir. Additional simulations were performed assuming a mixed boundary condition, where a heat transfer coefficient of 25 W/m^2 K representative of free convection and effective radiation heat transfer on the surface of the inertance tube with respect to a 300 K ambient environment. Most of the simulations were performed using the k - ω turbulence model in Fluent™, so comparison simulations were performed using the k - ε model of turbulence to compare the effect of these two standard turbulence models available in Fluent™ against experimental results.

The solver parameters used in Fluent™ included using the unsteady 2nd order model, the pressure-based coupled algorithm, PRESTO pressure based solver, the PISO scheme for pressure-velocity coupling, second order upwind for the momentum, temperature, turbulence model parameters and the QUICK scheme for density. A uniform quadrilateral mesh (meshing described above) was used for the inertance tube modeled as a cylinder in 2-D axisymmetric flow for the experimental tube[8] which is 2.357 m long with a diameter of 5.7 mm. The working gas was chosen as ideal helium and the wall chosen to be stainless steel, whose parameters are described by Fluent's material library. The boundary conditions for the wall were either isothermal or adiabatic as described above. The temperature of the tube is initialized to be 300 K and pressure to 2.5 MPa. The under-relaxation parameters were 0.5, 0.5, 0.9, 0.6, and 0.9 for the pressure, density, body-force, momentum and temperature, respectively. The residual convergence parameters were 1e-5, 1e-5, 1e-5, 1e-8, .01 and 1e-5 for the continuity equation, x-velocity, y-velocity, energy, turbulence kinetic energy (k) and turbulence parameter (specific dissipation rate ω or dissipation rate, ε depending on the model simulated). The max number of iterations is set at 500 for each time, with one cycle of a 60 Hz period meshed into 800 time steps.

To understand the convergence issue,[10-15] simulations were performed to look at the issue of time step size relative to mesh space size. This will aid the user in understanding the minimum required time steps size for the inertance tube modeled herein, but should not be construed as a requirement for other PTR component CFD modeling.

In this and the previous study our reduced order model of the inertance tube is compared to the experimental[9] and CFD data. The inertance tube reduced order model uses a friction factor based on steady flow and contains coefficients that can be adjusted. In this study, the possibility of adjusting these coefficients was investigated. To enable grid convergence studies and the scope of simulations of this study, the usage of High Performance Computing (HPC) Resources were used.

MODELS OF THE INERTANCE TUBE AND RESERVOIR

In the previous study, grid convergence techniques were presented to enable a better understanding of the errors associated with numerical simulations. This study presents the error bars associated with various simulations from the last study, as well as some new simulations. The previous CFD studies focused on a model of the inertance tube, where the reservoir is not meshed, but is simulated with a function that accounts for the mass flow into and out of the inertance/reservoir junction. This study expands on this mass flow function, by looking at the error bars via grid convergence techniques. This study meshed the reservoirs so that no user defined function was needed, and thus a complete mesh was done for both the inertance tube and the reservoir. In addition, this study looked at the effect of using a mixed boundary condition on the surface of the inertance tube wall. The previous studies used successive ratio meshes (which get finer the closer that the mesh gets to the wall), but in this study a uniform mesh was used. The previous study had a very course mesh in the axial direction and thus an extremely poor aspect ratio, in this study the meshing is very nearly equal in size for both the axial and radial directions and thus a nearly unitary aspect ratio. Due to the aspect ratio of this simulation the mesh size for the inertance tube for the coarsest grid yielded 26,400 nodes and for the next finest mesh 105,600 nodes and 422,400 nodes for the finest mesh. The emphasis of this study was understanding the effect of meshing small reservoir sizes including CFD of an inertance tube with no reservoir and thus the drawback of using an uniform mesh was large computation time but for doing this type of grid convergence study[18] it was convenient to use uniform mesh size. An adaptive mesh could have been used to reduce mesh in the reservoir and inertance tube, but would complicate this particular grid convergence study, as a different GCI methodology[11] would need to be used. The HPC center was used due to the large node counts. Many of the simulations where run from 2 up to 64 processors, with one of the 64 processor runs taking over 83 hours to yield 6 cycles worth of data! This particular run cost over 5300 hours worth of computational time. Testing was done to see what mesh/processor combination yielded the best times. In many cases, one could choose to optimize run time or computational time and we chose computational time, as this is what is allotted to us by the HPC.

This study meshed inertance tubes with reservoirs of size 0, 1, 30 and 334 cm^3 (the 0 cm^3 reservoir being just a capped or closed inertance tube on the reservoir side). The 30 cm^3 reservoir was the starting point for doing a grid convergence mesh doubling study and looked at meshes with a radial division of 16, 32 and 64 (with a nearly uniform mesh in the axial direction). The simulation with 64 radial divisions would not even run, and would crash, implying that the time step size was too big, and was the first hint of a CFL issue. Since this was a grid convergence doubling study, we halved the coarsest mesh (16 divisions) to get one with 8 radial divisions, and used the 8, 16 and 32 division simulations to come up with the grid convergence index (GCI-or error bar), solution method order (p) and the Richardson extrapolation (or the extrapolation to the ‘continuous’ solution). It should be noted that we compared two different grid convergence techniques, Pat Roaches’s[11] techniques and those of the JFE.[12] The finest grid with 32 divisions turned out to require the previously mention ~5300 hours of computation time. The next doubling to 64 radial divisions would not solve and thus implies that the spatial discretization size for the CFL condition with respect to the chosen time step size is bounded between 32 and 64 divisions. Since we had limited HPC computational hours, the other reservoir sizes (and other simulations of this study) were not all simulated on three successively doubling grids. The result was that a two grid convergence study was done for many of the other simulations. The drawbacks of using the two grid (instead of the three grid) technique is that the order of the method cannot be derived, no asymptotic convergence verification of the solution, and potentially a worse Richardson extrapolation to the continuous solution.[18] Since the order of the method cannot be verified for the two grid technique, the order of the method must be assumed which impacts the error bar estimate, as the error bar estimate is a function the solution method’s order. So from the equations in the previous study[7] (5) thru (10), the order (p) is assumed and results calculated based on this order assumption. It should be pointed out that for the two grid method that both Pat Roache’s[11] technique and the JFE[12] technique are identical. In Fluent many of the solvers are at least second order, some of them are fourth and some are not stated, so having the three grid method to determine the order of the solution methods can be very vital when predicting errors, but has potential pitfalls[16]. In previous studies as well as for the 334 cm^3 reservoir of this study, the acoustic power was seen to go from 234.33 W for the coarsest mesh to 233.95 W for the middle mesh and to 234.30 W for the finest mesh. While these values are indeed very close to one another this simulation does not show monotonic convergence.[11,15] If one only had two of these meshes (i.e. the coarsest and middle mesh) and attempted to extrapolate, one would get a different answer than extrapolating with a different set of two (i.e. the middle and the finest mesh).

The main metrics studied in this simulation are the phase shift between mass flow rate and pressure and the acoustic power. These are the only metrics of this study as the purpose of this work is to find out whether reduced order and high order methods like CFD are capable of predicting correctly phase shift and acoustic power. It should be noted that both of these quantities are area weighted quantities that come out of Fluent™ which are then time integrated as shown in the previous study equations[8] (3) and (4). We have used the conventional area weighted quantities to report the results of the study. It should be pointed out that mass weighted quantities could be also used in grid convergence studies. Boole's rules was used to evaluate the integrals, which is an eighth order (in time, in this case) method, so the integration error should be O(time step size=2e-5)[6] or approximately 10^{-28}, much better than machine epsilon. There are only six or eight significant digits in the pressure and mass flow rate output of Fluent, so there is probably more truncation error due to the output data format than due to the integration error. Many other metrics are possible when trying to validate the solution, with the conservation values probably being the best target metrics. Since phase shift and acoustic power are derived from these conserved quantities, if one finds they don't predict well, then the conserved quantities should probably be looked into more thoroughly. The ability to predict the correctness of metrics should be done with an understanding of what the associated numerical analysis errors are when solving the oscillating flow problem in Fluent™. For example to make the statement that mass streaming has been seen in Fluent, requires very stringent numerical errors based on the solution technique. Once the numerical analysis errors are better understood, with respect to the physical phenomena studied, then one can begin to have better confidence to make statements about the phenomena involved. To that end we present the results of our study with emphasis placed on the error bars calculated from various grid convergence techniques. In addition, the mixed boundary condition on the tube surface was included in the simulation representing the conjugate heat transfer that actually occurs in applications.

SIMULATION RESULTS AND DISCUSSION

The comparisons of acoustic power are shown in Figure 2 and phase shift are shown in Figure 3. In this two figures it should be noted that because of the nature of the log plots, that the zero cm^3 reservoir is plotted as a .1 cm^3 reservoir (10^{-1}). Compared in these figures are the (a) results from experiments at NIST,[8] with the various numerical simulations, including (b) the fully meshed inertance tube/reservoir system, the simulations (c) with just a meshed inertance tube with

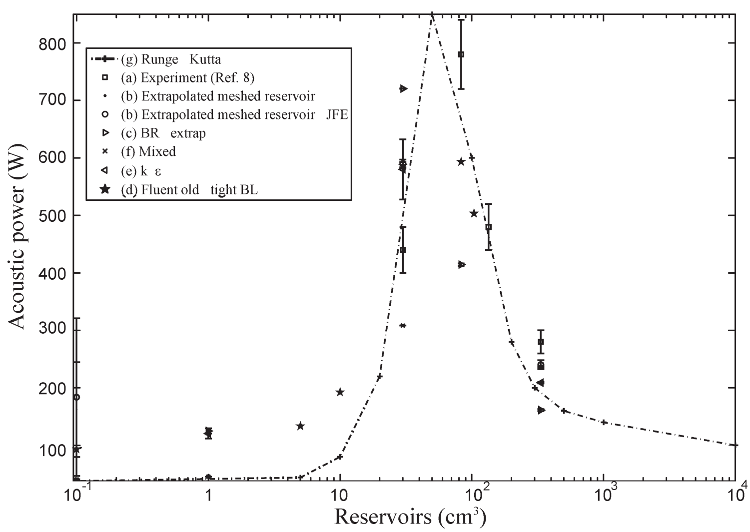

Figure 2. Comparison of acoustic power between different models and NIST experimental results.[8] For most of the simulations, the size of the error bar is equal to the size of the symbol and thus appears as solid symbols.

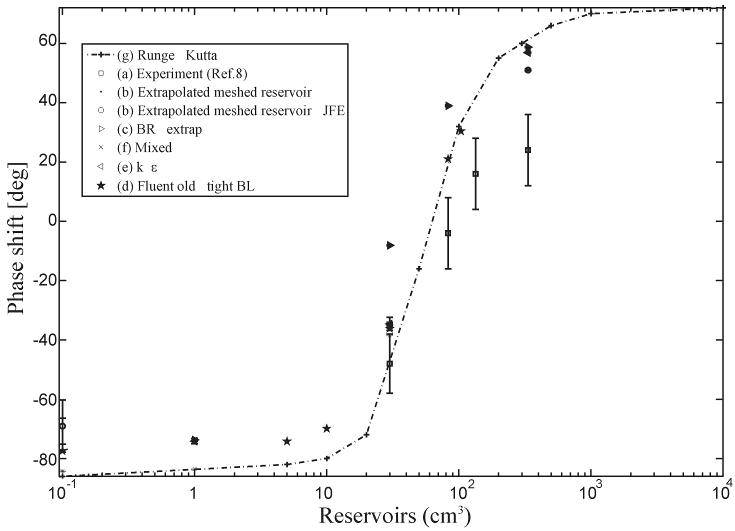

Figure 3. Comparison of phase shift between different models and NIST experimental results.[8] For most of the simulations, the size of the error bar is equal to the size of the symbol and thus appears as solid symbols.

the user defined function for the reservoir, (d) the previous studies results (same as (c) but much coarser in the axial direction, and successive ratio in the axial direction), (e) results (all others were simulated with), and (f) mixed boundary condition simulations, and finally (g) our Runge-Kutta reduced order method. Where applicable, the two methods for the three grid convergence techniques are shown in the figures, and as only one for the two grid techniques (as stated above that the two techniques become identical). As can be seen in these simulations, none of the CFD simulations for the acoustic power or phase shift and their calculated error bars overlapped with any of the NIST experiments and their associated error bars. The closest these came was with the acoustic power for the 30 cm^3 reservoir. It should be pointed out that important efforts in experimental validation of CFD have been undertaken and should be continued.[16,17] We have found it convenient to use the NIST experiments for comparison.[8] It should also be noted that there were very large error bars for the capped inertance tube (0 cm^3 'reservoir'). What is encouraging from these simulations was that the comparisons where fairly close for the fully meshed inertance tube and reservoir to that of the meshed inertance tube with the user defined function for the reservoir. This would imply that one could use the simplified reservoir function which is less costly computationally than that of meshing up fully the reservoir.

There were many interesting phenomena reported previously[18-20] that were seen in this study as well, including the change in pressure as a function of inertance tube length and reservoir size. A sample of pressure and mass flow variations with time are shown in Figure 4. One can see as the reservoir size increases that the pressure begins to act more like it does for steady flow. This may be a resonance statement, and one would desire an ability to understand mathematically this functionally with respect to the inertance tube, reservoir and operating conditions.

The next simulation data collected was the comparison of the isothermal boundary conditions to that of the mixed boundary conditions on the tube surface. Shown in Figure 5 are samples of temperature, pressure and mass flow rate in the fluid for these two different boundary conditions for different reservoir sizes as a function of inertance tube length. The results for tubes in this study show that the mixed boundary conditions affect the smaller reservoirs to a much greater extent than the larger ones.

Table 1 shows the spatial grid convergence index (GCI) tests and results as well as the order of convergence (p). The spatial GCI represents the error bar and should be understood as the percent error of the simulation value. The order of convergence should represent the order of the solver,

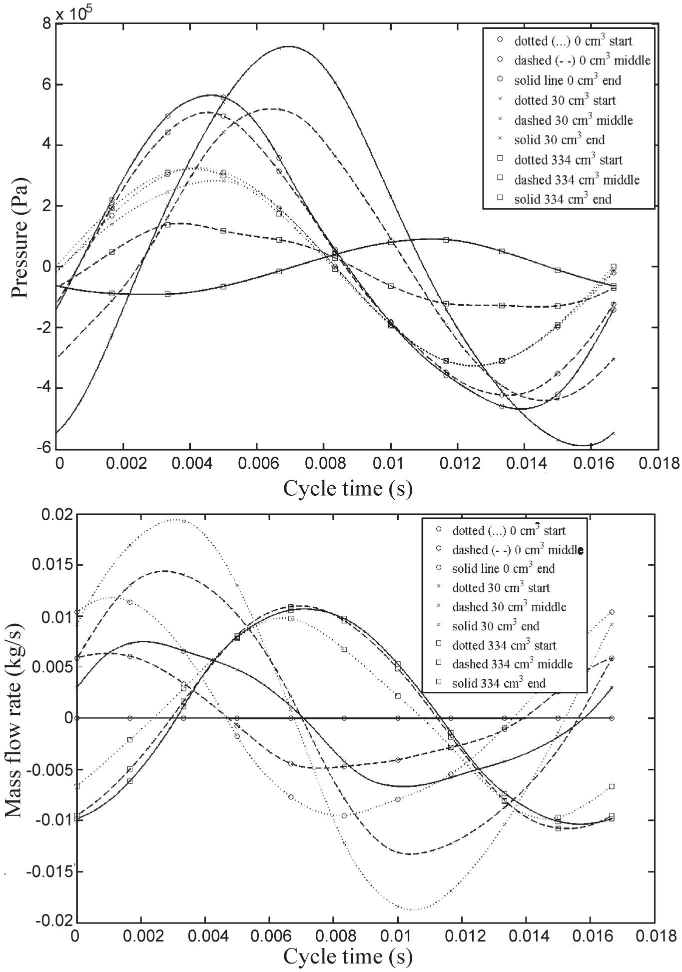

Figure 4. (Top) Pressure as a function of tube length for different reservoirs, (Bottom) mass flow rate as a function of tube length for different reservoirs.

where as mentioned above, the three grid technique allows one to calculate the order of the simulation method, otherwise for the two grid technique the order must be assumed, and thus impacts the error bars placed on the simulation value. One cycle of data consists of 800 time steps and many of these simulations did not run for the desired six cycles. The GCI and order p were calculated at the number of time steps shown in the table and was chosen as the minimum number of steps from the two or three mesh doublings simulated. For example the coarsest mesh may have run for 4801 time steps, the middle (or halved mesh sizes) mesh ran for 1501 steps and the finest mesh (again halved) ran for 3233 steps, then the comparison is done for the minimum of these (1501 steps). A more fair comparison in the table would have taken the minimum of all of the simulations, but the table shows that GCI and order can be calculated at any time during the simulation. For the B. Flake's reservoir function[12] at 30 cm^3, the three grid technique was applied but two grid techniques are shown for comparison purposes in the two tables above. Taking the 30 cm^3 example, if a two grid technique was simulated and one assumed the simulation method order to be two for calculating the phase shift, the three grid technique shows the order to be .55 and the order for acoustic power to be 4.93. One would then be under-estimating the errors by assuming a second order solution method for the phase shift and over-estimating the errors for the acoustic power. The GCI and order can be

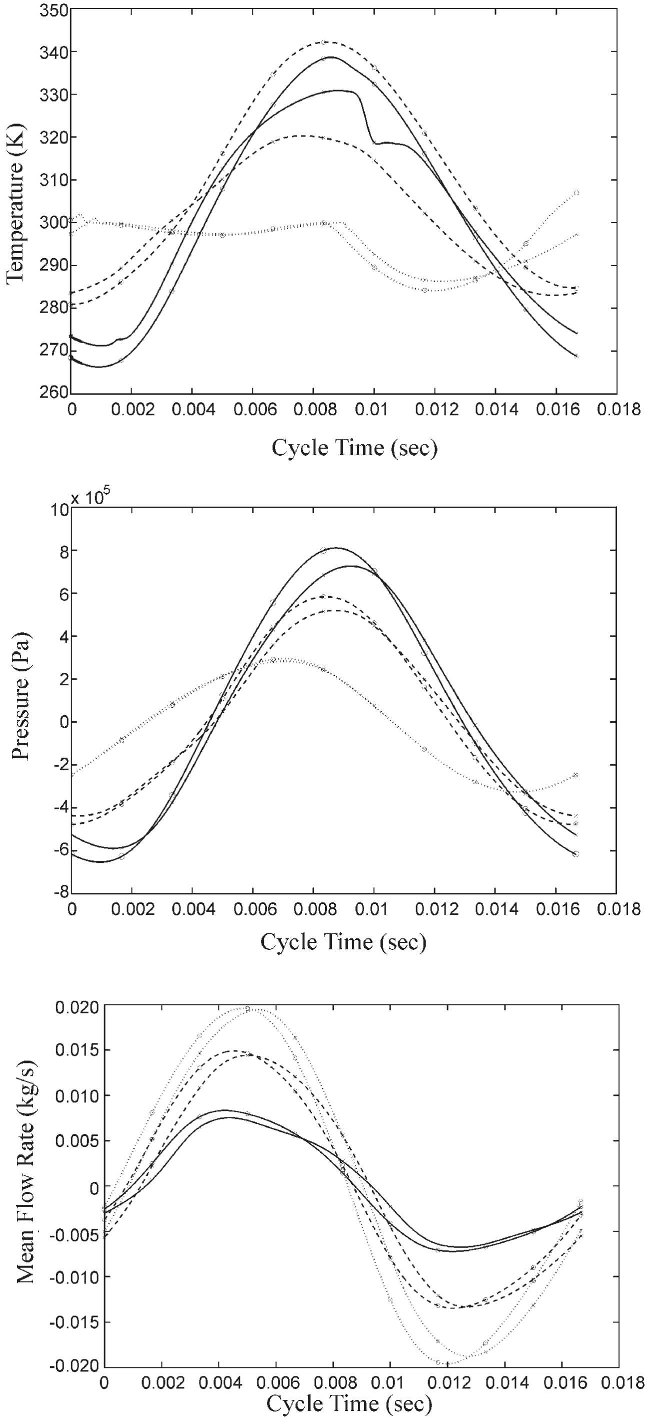

Figure 5. Sample results as functions of tube length for a 30 cm^3 reservoir: (Top) Temperature, (Middle) Pressure, (Bottom) Mass flow rate The circles represent the mixed case, while the x represents the isothermal boundary condition case. The dotted (…) line represents the beginning of the tube, the dashed line (- -) the middle of the tube and the solid line the end of the tube (nearest the reservoir).

Table 1. The two tables list the results of two and three grid convergence tests. Shown are grid convergence tests and grid convergence index (GCI) and convergence order (p) results for the acoustic power (AP) and the phase shift (PS) for the k - ε and k - ω models, reservoir function used in Flake and Razani.[4]

Two grid convergence tests and results

Reservoir	Model	Time steps	GCI, p=.5 PS	GCI, p=1 PS	GCI, p=2 PS	GCI, p=4 PS	GCI, p=.5 AP	GCI, p=1 AP	GCI, p=2 AP	GCI, p=4 AP
0 cm^3	$k-\varepsilon$	1956	.0347	.0144	.0048	9.6e-4	.2083	.0863	.0288	.0058
0cm^3-mixed	$k-\omega$	4297	.0017	7.1e-4	2.4e-4	4.7e-5	.0178	.0074	.0025	4.9e-4
1 cm^3	$k-\omega$	2082	.0895	.0371	.0124	.0025	.5217	.2161	.0720	.0144
1 cm^3	Br-$k-\omega$	3188	.0431	.0179	.0060	.0012	.2657	.1100	.0367	.0073
30 cm^3	Br-$k-\omega$	1501	.1331	.0551	.0184	.0037	.0033	.0014	4.6e-4	9.1e-5
30 cm^3	$k-\varepsilon$	1451	.0895	.0371	.0124	.0025	.5217	.2161	.0720	.0144
83 cm^3	Br-$k-\omega$	1516	.0503	.0208	.0069	.0014	.0405	.0168	.0056	.0011
334 cm^3	$k-\varepsilon$	1504	.0229	.0095	.0032	6.3e-4	.0463	.0192	.0064	.0013
334 cm^3	Br-$k-\omega$	1646	.0210	.0087	.0029	5.8e-4	.0720	.0298	.0099	.0020

Three grid convergence tests and results

Reservoir	Model	Time steps	GCI-PS/JFE	GCI-AP/JFE	Order-PS/JFE	Order-AP/JFE
0 cm^3	$k-\omega$	4801	.0616/.0906	.5092/.7461	.1844/.1278	.1428/.0990
30 cm^3	$k-\omega$	4801	.0170/.0267	.0077/.012	.7655/.5306	.643/.4457
30 cm^3	Br-$k-\omega$	1501	.0492/.0756	1.9e-5/3.7e-4	.5525/.3830	4.93/1.34
334 cm^3	$k-\omega$	4801	.0029/.0048	8.4e-5/.032	1/.6931	4.53/.0822

calculated for any simulation values (like mass flow rate, pressure, temperature, etc…), including the integrated quantities like the acoustic power and phase shift (which are integrated or Fourier transformed). Thus the values for GCI and order for these integral quantities can imply that there are issues with the raw data manipulation techniques.

The metrics chosen for determining whether k - ε or k - ω are better is not readily apparent in this study. In the previous studies it was found that mass conservation values are closer to what is desired for k - ω, but without an understanding of the grid convergence issues for either technique, it is nearly impossible to identify whether one technique predicts values better than the other. One of these techniques may be better at validating the mass flow rate and the other at validating the pressure for an experiment. Determining whether the validation of the simulation is correct needs to be less subjective and in the above example, should be based on numerical analysis techniques applied to the simulation solution methods. It would be incorrect to state that this study validated the simulation results at 30 cm^3 with the experiment, while recognizing the large and small reservoir results don't correlate as well to the experiment. It could purely be coincidence that the 30 cm^3 simulation results were good and incorrect to expect the large reservoir correlation to be as good as the 30 cm^3 results. In the case of the large reservoir, the error bars for the simulation and experiment do not overlap, so if the GCI is good (or small) then there are only a few options for trying to get a better simulation correlation. These include trying different solvers, trying different time step size (and thus mesh sizes), different iteration criteria, different data manipulation techniques, different turbulence solvers and turbulence or heat transfer boundary conditions. With each of these issues, grid convergence techniques will at least yield an ability to quantify error bars and solution convergence orders.

Based on Eqn. (4) in the previous study,[8] a sensitivity analysis was performed on the three coefficients, a_1, D_1 and D_2. The sensitivity analysis verified that a_1 was insensitive, while the other two coefficients were much more sensitive to change. Sensitivity analysis was done for the small 30 cm^3 reservoir and for the large 334 cm^3 reservoir. The results showed that for both of these reservoir sizes that various combinations of D_1 and D_2 would not yield results correlated to experiment for both of the values of acoustic power and phase shift.

CONCLUSIONS

Validation and verification (V&V) are complex issues especially when correlating experimental data to a simulation. In the case of using a simulation to obtain numerical solutions for oscillating flow in cryocooler components, the complexity of V&V is enormous. In this study, an attempt has been made to show how to obtain the error bars associated with doing grid convergence studies. The error bars from the CFD studies did not overlap those of the experiment. Thus there are many things to question in this study when attempting to make any V&V correlation statements. These questions include the use of area weighted values instead of nodal values when comparing mass flow rates, pressures and temperatures. The CFL[11] value, which is a functional measure of the time step size compared to the space step size, could be too tight or even to loose, requiring grid or time coarsening or refinement. The k - ε and k - ω models have values for inlet and outlet kinetic energy that are constant (set internally by Fluent: though the user can change them), and may thus represent stringent or unrealistic values for these oscillating flow studies. The solution methods may not be high enough to give accurate results. The iteration criteria may not be low enough or the under-relaxation values may be incorrect. There are many issues that could affect the poor correlation to the experiment, and only a systematic effort will yield a proper understanding of the issues. Future studies will focus on a systematic understanding of how to better simulate the required grid convergence needed to complete a successful V&V.

This study revealed that the user defined function for the reservoir provided a decent correlation with the meshed reservoir results. It would be far-flung to assume that one worked better than another for all inertance tube and reservoir combinations. The results from the mixed boundary condition on the surface of the tube showed that the larger reservoir was less sensitive to this boundary condition than the smaller reservoir. Again, it would not be wise to assume that this is the case for different sized tubes and reservoirs. Further studies will focus on these issues as functions of inertance tube and reservoir dimensions.

The friction factor results need more computation to elucidate whether the current friction factor method will yield good predictions for phase shift and acoustic power.

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